

# Supplementary Information

## Mechanisms of soil organic carbon and nitrogen stabilization in mineral associated organic matter – Insights from modelling in phase space

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### 10 S1. Generalized model including dissolved organic matter dynamics

C and N are transferred between POM and MAOM compartments partly via dissolved organic matter (DOM), which is only considered implicitly in the model presented in the main text (Fig. 1). In this appendix, we present a more general model including a DOM compartment, and show which simplifications lead to the model used in the main text. To construct this more general model, we assume that a fraction of the depolymerized products from POM and MAOM are used locally by the  
15 respective microbial communities (fractions  $1 - l_P$  and  $1 - l_M$ , respectively) and a fraction is transferred to a ‘shared’ DOM compartment (fractions  $l_P$  and  $l_M$ , respectively). DOM is then taken up by both communities according to the rates  $U_P$  and  $U_M$  (Fig. S1).

The C mass balance equations for the substrate (second subscript  $S$ ), microbial biomass (second subscript  $B$ ) in the POM (first subscript  $P$ ) and MAOM (first subscript  $M$ ), as well as for the DOM (subscript  $D$ ) can be written as,

$$\frac{dC_{PS}}{dt} = - \underbrace{(1 - l_P)D_P}_{\text{uptake}} - \underbrace{l_P D_P}_{\text{POM} \rightarrow \text{DOM}} + \underbrace{(1 - m)M_P}_{\text{recycled mortality}}, \quad (1)$$

$$\frac{dC_{PB}}{dt} = \underbrace{e_P U_P}_{\text{growth on DOM}} + \underbrace{(1 - l_P)e_P D_P}_{\text{growth on POM}} - \underbrace{M_P}_{\text{mortality}}, \quad (2)$$

$$\frac{dC_{MS}}{dt} = - \underbrace{(1 - l_M)D_M}_{\text{uptake}} - \underbrace{l_M D_M}_{\text{MAOM} \rightarrow \text{DOM}} + \underbrace{m M_P}_{\text{in vivo}} + \underbrace{M_M}_{\text{mortality}}, \quad (3)$$

$$\frac{dC_{MB}}{dt} = \underbrace{e_M U_M}_{\text{growth on DOM}} + \underbrace{(1 - l_M)e_M D_M}_{\text{growth on MAOM}} - \underbrace{M_M}_{\text{mortality}}, \quad (4)$$

$$\frac{dC_D}{dt} = \underbrace{l_P D_P}_{\text{POM} \rightarrow \text{DOM}} + \underbrace{l_M D_M}_{\text{MAOM} \rightarrow \text{DOM}} - \underbrace{(U_P + U_M)}_{\text{uptake}}. \quad (5)$$

20 The rate of uptake of DOM by the POM microbes is probably smaller than the uptake by MAOM microbes, as the former primarily feed on POM substrates (i.e.,  $U_P \approx 0$ ). Moreover, we can assume that the DOM compartment is in quasi-

equilibrium (i.e.,  $dC_D/dt \approx 0$ ) because it is a small C compartment with relatively fast turnover rates. Mathematically, this means that  $U_M \approx l_p D_p + l_M D_M$ , which allows simplifying Eq. (1)-(5) and obtain the model described in the main text (after re-naming  $l = l_p$ ).

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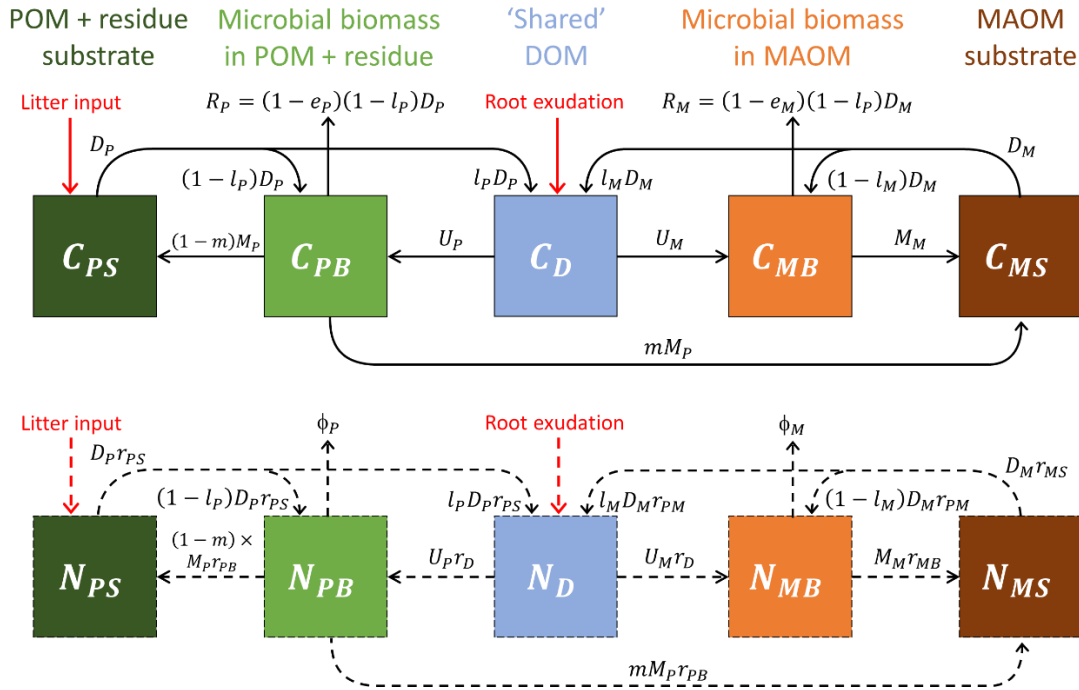


Figure S1. Schematic of the generalized model including a dissolved organic matter (DOM) compartment. Solid and dashed arrows or compartment edges indicate respectively C and N flows or compartments. Plant input rates to POM (litter) and DOM (root exudates) are shown as red arrows, but are not included in the model equations because a single cohort of residues is tracked during decomposition and stabilization.

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## S2. General solutions for partly soluble residues ( $b < 1$ )

The following equations are the general solutions of Eq. (10) (for  $c_M(c_P)$ ) and (24) (for  $n_P(c_P)$ ) in the main text when the added residues are partly soluble ( $b < 1$ ),

$$c_M = \frac{c_P \left( l + \frac{am}{1-m} \right) + \left( \frac{c_P}{b} \right)^{\frac{\kappa(1-e_M)}{1-a}} \{ (1-b)[\kappa(1-e_M)-1] - bl + a \left( 1 - \frac{b}{1-m} \right) \}}{\kappa(1-e_M) + a - 1}, \quad (6)$$

$$n_P = c_P \frac{r_B}{r_0} + \left( 1 - \frac{r_B}{r_0} \right) b \left( \frac{c_P}{b} \right)^{\frac{1}{1-a}}. \quad (7)$$

The full analytical solution of Eq. (26) for  $n_M(c_P)$  is rather cumbersome and less mathematically insightful, so we do not report it here. These equations can be simplified as done in the main text by substituting  $a = e_P(1-l)(1-m)$ , simplifying where possible the factor  $1-m$ , taking the limit for  $m \rightarrow 1$  (as motivated in Section 3.2), and further assuming that all microbes have the same CUE ( $e$ ). These simplifications lead to the more compact solutions,

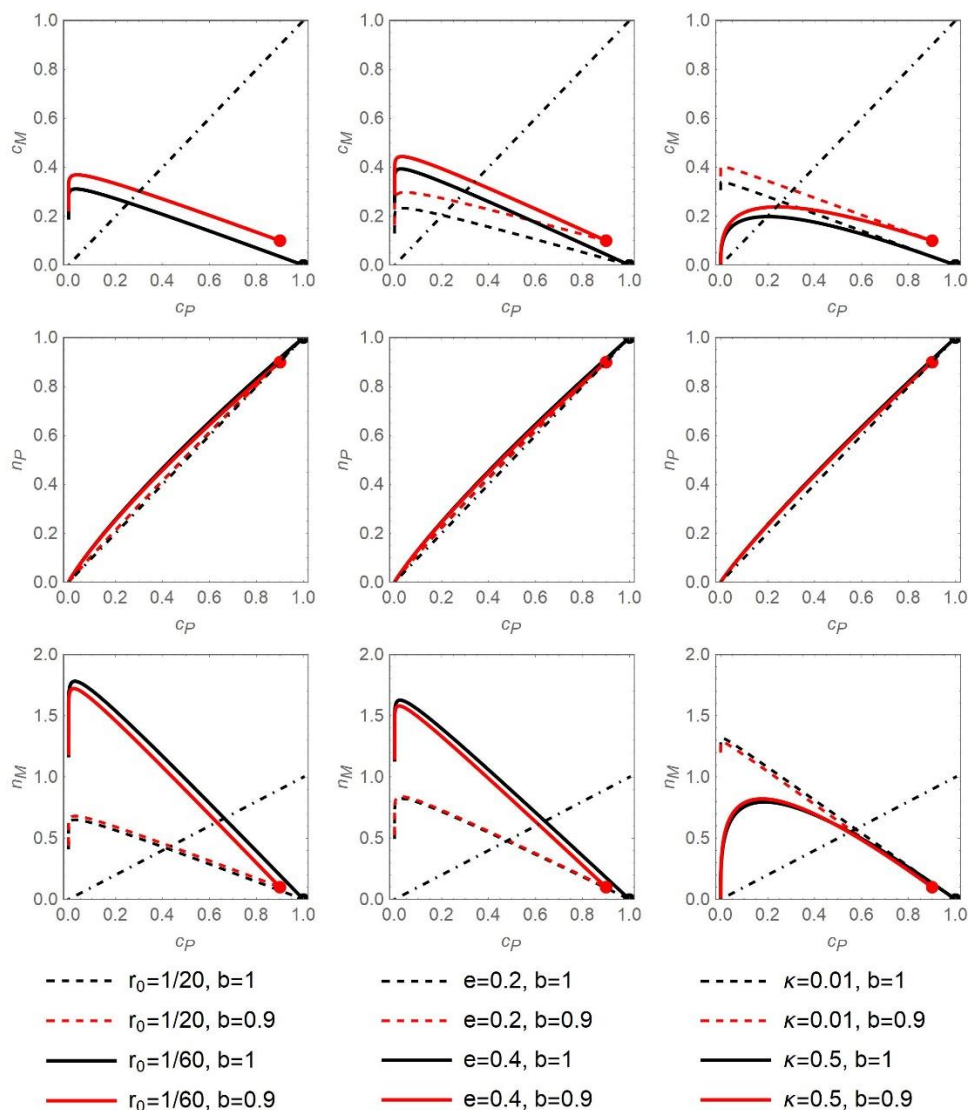
$$c_M = c_P \frac{l(1-e)+e}{\kappa(1-e)-1} + \left( \frac{c_P}{b} \right)^{\kappa(1-e_M)} \left\{ 1 - b \left[ 1 - \frac{l(1-e)+e}{\kappa(1-e)-1} \right] \right\}, \quad (8)$$

$$n_P = c_P, \quad (9)$$

$$n_M = c_P \left[ l - \frac{(\kappa+l-1)e}{1-\kappa(1-e)} \frac{r_B}{r_0} \right] \frac{1}{\kappa-1} + \left( \frac{c_P}{b} \right)^\kappa \left[ 1 - \frac{b(\kappa+l-1)}{\kappa-1} \right] \left( 1 - \frac{r_B}{r_0} \right) + \left( \frac{c_P}{b} \right)^{\kappa(1-e)} \left[ 1 + \frac{b(\kappa+l-1)(1-e)}{1-\kappa(1-e)} \right] \frac{r_B}{r_0}, \quad (10)$$

with boundary conditions  $c_M(b) = 1 - b$ ,  $n_P(b) = b$ , and  $n_M(b) = 1 - b$ .

Fig. S2 illustrate the effect of residue solubility, mathematically represented by the parameter  $b$ . Compared to insoluble residues ( $b = 1$ ), residues whose fraction  $1 - b$  is immediately stabilized in MAOM have initial conditions at lower  $c_P$  and  $n_P$ , but correspondingly higher  $c_M$  and  $n_M$  levels (red circles in Fig. S2). Despite these different initial states, the trajectories of  $c_M$ ,  $n_P$ , and  $n_M$  in phase space generally converge to those of residues with  $b = 1$  as decomposition progresses. However, lower values of microbial CUE (low  $e$ ) and when MAOM is decomposed much slower than POM + residues (low  $\kappa$ ) cause the trajectories of  $c_M$  to remain separated for a longer period compared to the trajectories of  $n_P$ , and  $n_M$  (top panels in Fig. S2).



50 **Figure S2.** Fraction of added C in MAOM,  $c_M$  (top row), fraction of added N in POM + residues,  $n_P$  (center row), and fraction of  
 added N in MAOM,  $n_M$  (bottom row), as a function of the fraction of added C in POM + residues,  $c_P$ , at different levels of residue  
 55 solubility (colors) and when varying the values of model parameters: residue N:C ratio,  $r_0$  (left column), microbial carbon use  
 efficiency,  $e$  (center column), and ratio between the decay constants of MAOM and POM + residue decomposition,  $\kappa$  (right  
 column). Two solubility levels are considered: insoluble residues ( $b = 1$ ; black), and partly soluble residues resulting in rapid  
 stabilization of a fraction of residue ( $b = 0.9$ ; red). In all panels, residue decomposition progresses from right to left along the  
 curves, as  $c_P$  decreases; initial conditions are indicated by circles; the dot-dashed black lines indicate 1:1 lines, which represent  
 equality between the fractions of added C or N shown on the y-axes and  $c_P$  shown on the x-axes. Baseline parameters are:  $l = 0.1$ ,  
 $m = 0.9$ ,  $r_0 = 1/40$ ,  $e = 0.3$ ,  $\kappa = 0.05$ .

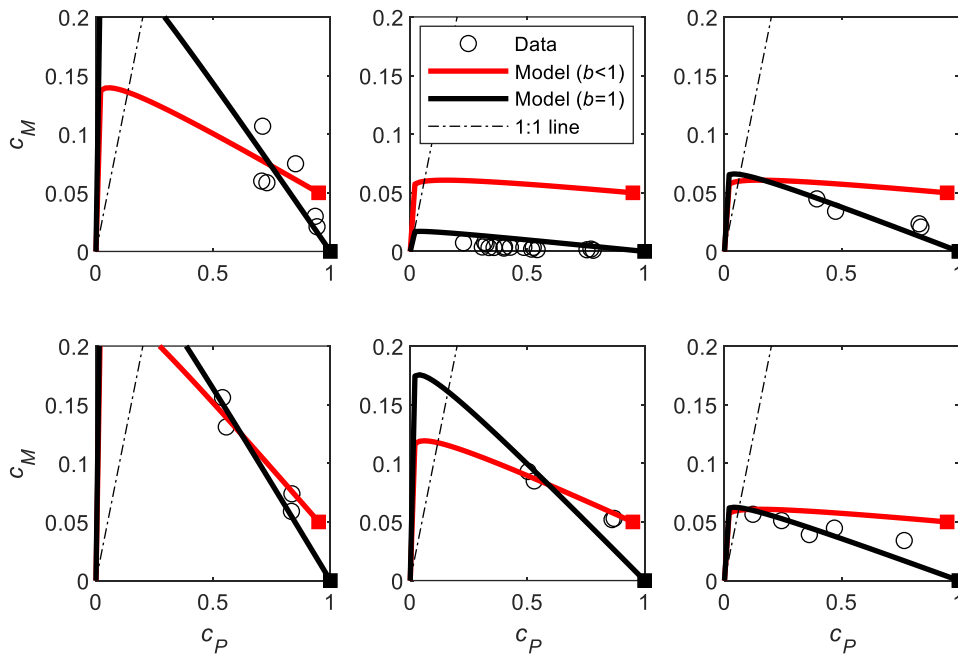
### S3. Comparison of models assuming insoluble ( $b = 1$ ) or partly soluble residues ( $b < 1$ )

To assess if model fitting improves when considering partial stabilization of soluble residues, we selected five datasets with sufficient resolution at the beginning of decomposition (when the effect of the initial condition is most relevant) and fitted two model versions: one with  $b = 1$  and one with  $b < 1$ . These five datasets (from four studies) tracked the fate of C from various types of grass and herb residues (Lavallee et al., 2018; Mitchell et al., 2018; Leichthy et al., 2021; Nunez et al., 2022). Assuming that ~10% of residue C is water soluble, and that approximately half of that can be readily stabilized, we obtain an estimate for  $b = 0.95$  (i.e., initial MAOM fraction is 0.05). For reference, ~20% of C in leachate can be stabilized as MAOM in one week (Even and Cotrufo, 2024), suggesting that the 50% figure we considered is at the high end of a reasonable range. In principle,  $b$  could be regarded as a fitting parameter as well, but most datasets lacked data points in the initial phases of decomposition (i.e.,  $c_p > 0.8$ ) so that  $b$  cannot be properly constrained. We could also estimate  $b$  from measured soluble C fractions for each residue type across the database, but these estimates would still be uncertain as we do not know how much of the soluble C is used locally by microorganisms in the POM + residue compartment and how much can be transported away and stabilized as MAOM. Therefore, we limit this model comparison to the two end-member cases of  $b = 1$  and  $b = 0.95$ .

The comparison between these two model versions is shown in Fig. S3. For some residue types, the measured fraction of added C in MAOM was much lower than 0.05, indicating that in those datasets very little soluble C was stabilized at the beginning of decomposition. In other datasets data seemed instead consistent with an initial fraction of added C in MAOM of about 0.05. Overall, the model assuming  $b = 1$  performed better than or comparably to the model assuming  $b = 0.95$  in five out of six datasets (lower or similar root mean square error). Therefore, considering the uncertainties around the value of  $b$  and lack of high frequency data to constrain the other model parameters, we can conclude that it is reasonable to assume  $b = 1$  across the database.

The parameters estimated with the two models were numerically different but highly correlated between models (Pearson correlation coefficients  $\geq 0.9$ ; Fig. S4). Specifically, the values of microbial CUE were slightly lower when assuming  $b < 1$ , while the fractions of depolymerized C stabilized as MAOM were much lower. This is expected because the two model versions are constrained to fit the same MAOM data. As a consequence, when more C is initially stabilized as MAOM ( $b = 0.95$ ), less C will be stabilized at later stages (lower  $l$ ). The high correlation between parameter values estimated with the two models suggests that conclusions on the significance and direction of the effects of soil and environmental drivers on  $e$  and  $l$  (Section 3.4 in the main text) are likely to be robust to variations in residue solubility.

More detailed studies of the fate of soluble C within days after the start of decomposition, or studies reporting MAOM at high frequency during the first days or weeks could provide constraints on the value of  $b$ . The equations reported in this Supplementary Materials are ready to be tested with such data.



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Figure S3. Fraction of added C in MAOM,  $c_M$ , as a function of the fraction of added C in POM + residues,  $c_P$ , at different levels of residue solubility (black:  $b = 1$ ; red:  $b = 0.95$ ) in five datasets where measurements during the early phase of decomposition ( $c_P > 0.75$ ) were available (Cotrufo et al., 2015; Lavallee et al., 2018; Mitchell et al., 2018; Leichty et al., 2021; Nunez et al., 2022). Curves are least square model fitting to the data using Equation (8) with  $\kappa = 0.05$  and  $e$  and  $l$  as fitting parameters (shown in Fig. S4). In all panels, residue decomposition progresses from right to left along the curves, as  $c_P$  decreases; initial conditions are indicated by filled squares; the dot-dashed black lines indicate 1:1 lines.

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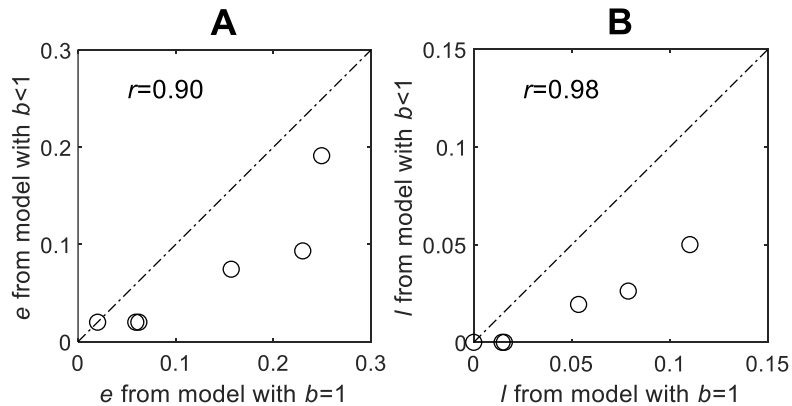


Figure S4. Comparisons between parameters estimated when assuming that the added residues were insoluble ( $b = 1$ , black curves in Fig. S3) or partly soluble ( $b = 0.95$ , red curves in Fig. S3): A) comparison of microbial C use efficiencies ( $e$ ) and B) comparison of fractions of depolymerized C stabilized in MAOM ( $l$ ). The dot-dashed black lines indicate 1:1 lines;  $r$ : Pearson correlation coefficients.

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## S4. Data

**Table S1. Sources and types of data.**

Data source	# treatments or sites	# residue types	residue source	# time points	C compartments				N compartments			
					residues	POM	residues + POM	MAOM	residues	POM	residues + POM	MAOM
Almeida et al. (2021)	1	4	P	1			×	×				
Antonio Telles Rodrigues et al. (2022)	5	1	P	1	×	×	×	×				
Buckeridge et al. (2022; 2021)	4	3	P, M	4			×	×			×	×
Canisares et al. (2023)	2	3	P	1	×	×	×	×				
Cheng et al. (2023)	1	4	P	3			×	×				
Cotrufo et al. (2015)	1	1	P	5	×	×	×	×	×			
Cotrufo et al. (2022)	2	5	P, O	1	×	×	×	×	×	×	×	×
Craig et al. (2022, 2021)	1	16	P	2	×		×	×				
Dai et al. (2022)	3	1	P	1			×	×				
Duan et al. (2023)	3	1	P	3		×		×				
Even and Cotrufo (2024)	4	1	P, O	2	×	×	×	×				
Fang et al. (2019)	12	1	P	2			×	×				
Ferreira et al. (2021), Oliveira et al. (2021)	2	2	P	2	×	×	×	×				
Fulton-Smith and Cotrufo (2019)	1	2	P	3	×	×	×	×	×	×	×	×
Haddix et al. (2020)	10	1	P	2			×	×				
Pries et al. (2017)	1	2	P	5	×	×	×	×	×	×	×	×
Pries et al. (2018)	3	1	P	3	×	×	×	×				
Huys et al. (2022a, b)	1	24	P	4	×	×	×	×				
Kölbl et al. (2007, 2006)	2	1	P	4		×		×		×		×
Kou et al. (2023b, a)	3	1	P	4	×	×	×	×				
Lavallee et al. (2018)	2	2	P	2			×	×			×	×
Leichty et al. (2021)	3	1	P	2	×	×	×	×				
Lian et al. (2016)	1	3	P	1	×	×	×	×				
Liebmann et al. (2020)	1	1	P	2	×	×	×	×				

Lyu et al. (2023)	1	2	P	2	×	×	×	×				
Magid et al. (2002)	1	1	P	3			×	×				
Mitchell et al. (2018)	4	1	P	4	×	×	×	×	×	×	×	×
Neupane et al. (2023)	6	1	P	3	×	×	×	×				
Nunez et al. (2022)	2	1	P	2	×	×	×	×	×	×	×	×
Nyamasoka-Magonziwa et al. (2022)	2	3	P, O	1		×		×				
Poeplau et al. (2023)	2	4	P	3			×	×				
Ridgeway et al. (2022)	2	4	P	1			×	×			×	×
Ridgeway et al. (2023b, a)	9	1	P	1			×	×			×	×
Schiedung et al. (2023)	11	2	P, O	1			×	×				
Sokol et al. (2019)	1	3	P	1		×		×				
Su et al. 2020	1	1	P	5		×		×				
Throckmorton et al. (2015)	2	1	M	5			×	×				
Wang et al. (2017)	1	4	P	4		×		×				
Xu et al. (2022)	4	2	P	1	×	×	×	×				

P: plant (leaves, shoots, roots, woody material), M: microbial necromass, O: other residues (e.g., manure, leachates)

105 ×: the data source includes some data points in the marked category, but not always in all treatment/site/residue type combinations



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